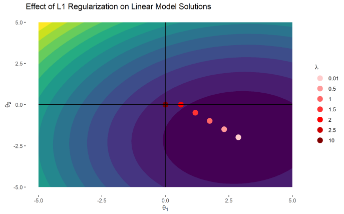
Introduction to Machine Learning

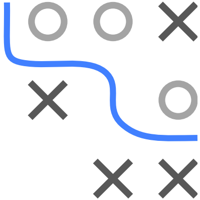
Regularization
Lasso Regression



Learning goals

- Lasso regression / $L1$ penalty
- Know that lasso selects features
- Support recovery

LASSO REGRESSION



Another shrinkage method is the so-called **lasso regression** (least absolute shrinkage and selection operator), which uses an $L1$ penalty on $\boldsymbol{\theta}$:

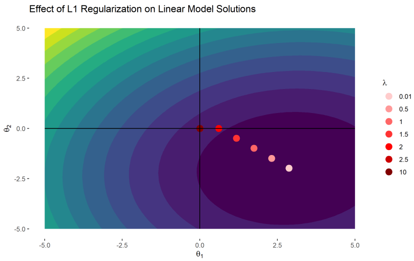
$$\hat{\theta}_{\text{lasso}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 + \lambda \sum_{j=1}^{p} |\theta_j|$$

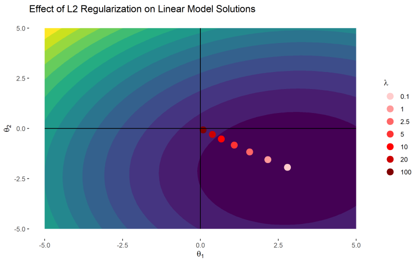
$$= \arg\min_{\boldsymbol{\theta}} \left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta} \right)^\top \left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta} \right) + \lambda \|\boldsymbol{\theta}\|_1$$

Optimization is much harder now. $\mathcal{R}_{\text{reg}}(\boldsymbol{\theta})$ is still convex, but in general there is no analytical solution and it is non-differentiable.

LASSO REGRESSION

Let $y = 3x_1 - 2x_2 + \epsilon$, $\epsilon \sim N(0,1)$. The true minimizer is $\theta^* = (3, -2)^T$. LHS = $L1$ regularization; RHS = $L2$

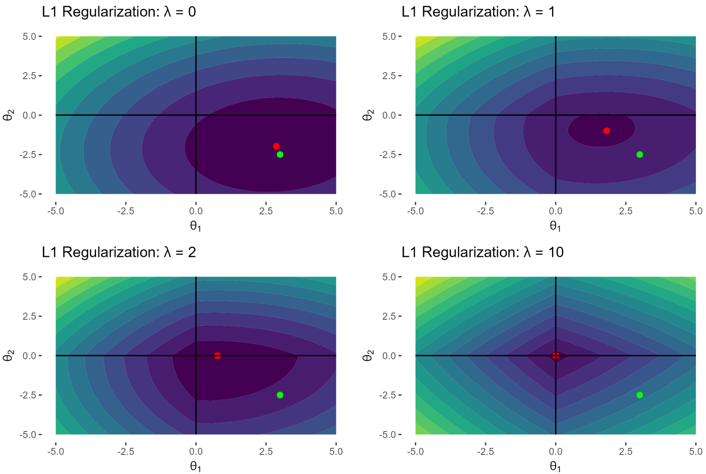




With increasing regularization, $\hat{\theta}_{lasso}$ is pulled back to the origin, but takes a different “route”. θ_2 eventually becomes 0!

LASSO REGRESSION

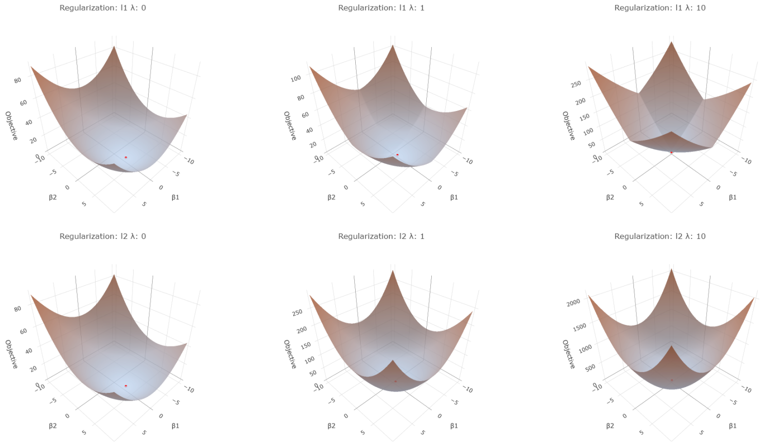
Contours of regularized objective for different λ values.



Green = true minimizer of the unreg.objective and red = lasso solution.

LASSO REGRESSION

Regularized empirical risk $\mathcal{R}_{\text{reg}}(\theta_1, \theta_2)$ using squared loss for $\lambda \uparrow$. $L1$ penalty makes non-smooth kinks at coordinate axes more pronounced, while $L2$ penalty warps $\mathcal{R}_{\text{reg}}$ toward a "basin" (elliptic paraboloid).

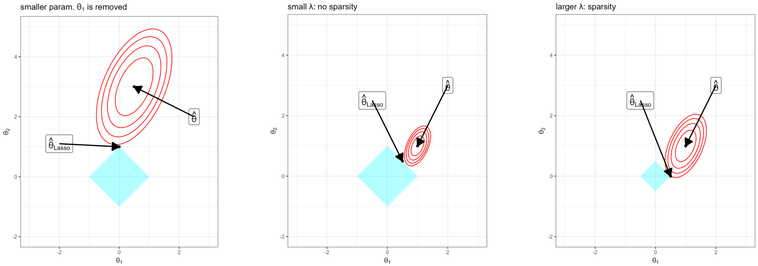


LASSO REGRESSION

We can also rewrite this as a constrained optimization problem. The penalty results in the constrained region to look like a diamond shape.

$$\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta} \right) \right)^2 \text{ subject to: } \|\boldsymbol{\theta}\|_1 \leq t$$

The kinks in $L1$ enforce sparse solutions because "the loss contours first hit the sharp corners of the constraint" at coordinate axes where (some) entries are zero.



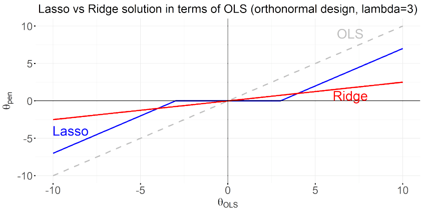
$L1$ AND $L2$ REG. WITH ORTHONORMAL DESIGN

For special case of orthonormal design $\mathbf{X}^\top\mathbf{X} = \boldsymbol{I}$ we can derive a closed-form solution in terms of $\hat{\theta}_{\text{OLS}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y} = \mathbf{X}^\top\mathbf{y}$:

$$\hat{\theta}_{\text{lasso}} = \text{sign}(\hat{\theta}_{\text{OLS}})(|\hat{\theta}_{\text{OLS}}| - \lambda)_+ \quad \text{(sparsity)}$$

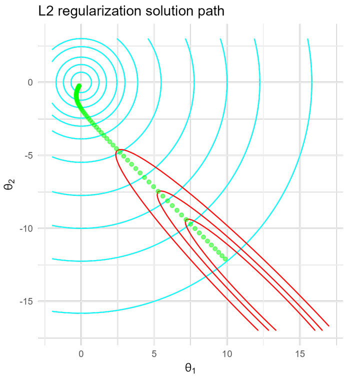
Function $S(\theta, \lambda) := \text{sign}(\theta)(|\theta| - \lambda)_+$ is called **soft thresholding** operator: For $|\theta| \leq \lambda$ it returns 0, whereas params $|\theta| > \lambda$ are shrunken toward 0 by λ.
Comparing this to $\hat{\theta}_{\text{Ridge}}$ under orthonormal design:

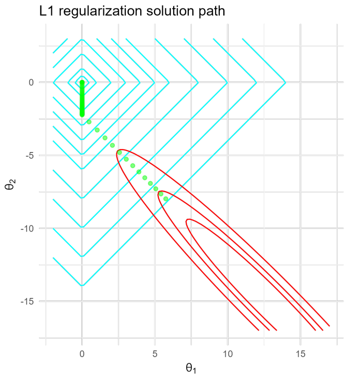
$$\hat{\theta}_{\text{Ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\boldsymbol{I})^{-1}\mathbf{X}^T\mathbf{y} = ((1+\lambda)\boldsymbol{I})^{-1}\hat{\theta}_{\text{OLS}} = \frac{\hat{\theta}_{\text{OLS}}}{1+\lambda} \quad \text{(no sparsity)}$$



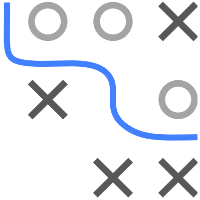
COMPARING SOLUTION PATHS FOR $L1/L2$

- Ridge results in smooth solution path with non-sparse params
- Lasso induces sparsity, but only for large enough λ





SUPPORT RECOVERY OF LASSO ▸ Zhao and Yu 2006



When can lasso select true support of $\boldsymbol{\theta}$, i.e., only the non-zero parameters?
Can be formalized as sign-consistency:

$$\mathbb{P}\big(\text{sign}(\hat{\boldsymbol{\theta}}) = \text{sign}(\boldsymbol{\theta})\big) \to 1 \text{ as } n \to \infty \quad (\text{where}\,\text{sign}(0) := 0)$$

Suppose the true DGP given a partition into subvectors $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ is

$$\boldsymbol{Y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\varepsilon} = \mathbf{X}_1\boldsymbol{\theta}_1 + \mathbf{X}_2\boldsymbol{\theta}_2 + \boldsymbol{\varepsilon}\,\text{with}\,\boldsymbol{\varepsilon} \sim (0, \sigma^2\boldsymbol{I})$$

and only $\boldsymbol{\theta}_1$ is non-zero. Let $\mathbf{X}_1$ denote the $n \times q$ matrix with the relevant features and $\mathbf{X}_2$ the matrix of noise features. It can be shown that $\hat{\boldsymbol{\theta}}_{lasso}$ is sign consistent under an **irrepresentable condition**:

$$|(\mathbf{X}_2^\top \mathbf{X}_1)(\mathbf{X}_1^\top \mathbf{X}_1)^{-1}\text{sign}(\boldsymbol{\theta}_1)| < \mathbf{1} \text{ (element-wise)}$$

In fact, lasso can only be sign-consistent if this condition holds.
Intuitively, the irrelevant variables in $\mathbf{X}_2$ must not be too correlated with (or *representable* by) the informative features ▸ Meinshausen and Yu 2009